NICEST GSAS/RIETVELD WORKSHOP

Saturday 15th March to lunchtime Sunday 16th March

Taught by:

- Ross Angel (Virginia Tech)
- Jason Hodges (SNS-IPNS)
- Brian Toby (NIST)
- Plus graduate student assistants from Virginia Tech, if needed

Purpose:

- Provide a basic understanding of the principles of fitting powder diffraction patterns by Rietveld and Le Bail techniques.
- Introduce the GSAS package of programs. By the end of the course participants will be able to define a crystal structure model for Rietveld refinement and to perform Rietveld and Le Bail fits with GSAS under the EXPGUI interface and interpret the results.

Requirements of participants:

- Basic knowledge of diffraction theory (Bragg's law; structure factor computation; Fourier maps).
- Basic computer operation skills for use of Windows or Linux.
- Participants may bring their own laptops on which to do GSAS exercises; bring a CDROM or Zip drive to load software.

Course organization:

In order to accommodate participants with a wide range of experience with Rietveld refinement, the course will consist of some overview lectures and a large number of hands-on exercises. The exercises range from those for absolute beginners to those for experts. Participants make their own selection of exercise(s) to perform during the hands-on course period. Course instructors will be available for guidance. Participants may bring their own laptops or use computers provided at the SNS.

Timetable

Saturday

08:30-09:30	Lecture: Introduction to ideas of Rietveld analysis (RJA)
09:30-10:30	Lecture: Overview of GSAS & EXPGUI (BHT)
10:30-11:00	Coffee break, discussions
11:00-lunch	Exercises
lunch	
lunch-15:00	Exercises
15:00-16:00	Lecture: GSAS parameters (BHT)
16:00-17:00	Lecture: Special issues with TOF data (JH)

Sunday

08:30-09:30	Lecture: Judging quality of Rietveld fits (RJA)
09:30-12:00	Exercises
12:30-13:00	Closing remarks and discussion

Background Reading and References

Attendees who are unfamiliar with Rietveld refinement are advised to obtain at least one of the first two references before the course.

"The Rietveld Method", edited by R.A. Young. *An excellent introductory guide to pattern fitting. Beginners are encouraged to read the first chapter, at a minimum. Available from the IUCr website:* http://www.iucr.org/

"Rietveld refinement guidelines" McCusker et al. *J. Appl. Cryst.* (1999) 32:36-50. *Another good beginner's guide.*

"Fundamentals Of Crystallography" C. Giacovazzo editor, (Oxford University Press, New York, 1992). *A good crystallography reference.*

Software

All of the software, datasets and other files used in the course will be provided on CD-ROM to participants.

GSAS is a suite of Fortran programs written originally for VAX computers. The code was subsequently ported to Unix and Windows. GSAS is freely available. To help support the continued development of GSAS you should provide appropriate acknowledgement in published work. The reference to the GSAS manual is: A.C. Larsen and R.B. Von Dreele (1985) Los Alamos National Laboratory Report LAUR B6-748. More details at http://public.lanl.gov/gsas/

GSAS programs obtain input in a question-and-answer mode that is supported on all computer platforms, but can be difficult for beginners to master. An alternative to this is a graphical user interface, EXPGUI, which implements many, but not all, of the features of GSAS. The EXPGUI interface will be used in this course. To support the continued development of the EXPGUI project, please reference: B. H. Toby, *EXPGUI*, a graphical user interface for *GSAS*, *J. Appl. Cryst.* (2001). **34**, 210-213. For information on EXPGUI see: http://www.ncnr.nist.gov/xtal/software/expgui/

NICEST PDF/DISORDERED MATERIALS HANDS ON COURSE WORKSHOP

(**To Be Announced)**